

OXIDATION OF NITROGEN OXIDE IN HOMOGENEOUS GAS PHASE REACTIONS: COMBUSTION EMISSIONS CONTROL MODELING

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Abstract

An analytical study on the oxidation of NO in homogeneous gas phase reactions is presented. Although NO is readily oxidized to NO₂ at room temperatures, the conversion rate falls with increasing temperature. However, aliphatic alcohols and hydrocarbons generate HO₂ which appears to oxidize NO at higher temperatures. In a medium containing oxygen and aliphatic alcohols or hydrocarbons, NO oxidizes to NO₂ even at 1000 K; but NO₂ returns to NO after these compounds are consumed. Various aliphatic compounds (ethane, butane, methanol, and ethanol) will be considered in this discussion. These chemicals may be useful in the treatment of emissions from stationary combustion systems for removal of NO_x.

Introduction

Nitrogen oxides (NO_x) pose serious environmental concerns due to their role in smog and acid rain formation.(1) These oxides are natural products of combustion, where high temperatures lead to their formation through reactions between dissociated nitrogen and oxygen (thermal NO_x) or through oxidation of nitrogenous compounds created during the combustion process (prompt NO_x). (2,3)

The extent of NO_x formation depends on the initial fuel/air mixture ratio, with greater amounts of NO_x generated with fuel-lean and stoichiometric mixtures. Thus, to control NO_x formation during combustion, one might be tempted to burn a fuel-rich mixture. However, this leads to excessive production of unburned hydrocarbons and carbon monoxide, which also pose severe environmental problems. All of these pollutants can be controlled through careful combustor design (4), but the resultant configuration may have other undesirable characteristics.

Post-combustion treatment of the exhaust to remove NO_x provides an alternative means of reducing the pollution problem. One method introduces various nitrogenous compounds (5-9) into the exhaust stream to react with the NO_x, reducing its concentration. However, this technique is limited to a narrow range of temperatures.(10)

Another post-combustion process removes the NO_x by scrubbing with water. Unfortunately, the poor solubility of most nitrogen oxides precludes direct application of this technique. NO_x is typically comprised of three species: NO, NO₂, and N₂O; and, although nitrogen dioxide (NO₂) is fairly soluble in water, nitrogen oxide (NO) predominates due to the high temperatures associated with combustion. To make the scrubbing technique feasible, the NO needs to be converted to NO₂.(1)

Lyon, et al, improved NO to NO₂ gas phase oxidation through treatment with methanol.(11) The present study expands on this theme by examining NO oxidation in the presence of methanol, ethanol, ethane, and butane.

Physical/Computational Models and Kinetics Mechanisms

Nitrogen oxides are indirect products of combustion, with the extent of formation dependent on temperature and residence time in the combustor. Although combustion is typically complete within a millisecond, NO_x in a fuel-lean mixture grows steadily with time as long as the temperature remains high. However, although equilibrium levels of nitrogen oxides are very high (Fig. 1), NO_x concentrations rarely reach these levels in conventional combustion processes. Thus, while the exhaust stream composition may approach equilibrium in general, the NO_x concentration will not.

The ability of hydrocarbons and alcohols to oxidize NO_x in an exhaust stream that, apart from the NO_x , is at equilibrium will be examined using the LSENS program of Bittker and Radhakrishnan.(12) In particular, the code's plug flow reaction model is used to compute concentrations at various times during the combustion process.

The starting point for these calculations will be the fuel-lean mixture described in Table I. As shown in the table, all of the NO_x is in the form of NO. This follows from the argument that, in the absence of hydrocarbon fragments, any NO_x present would be converted to NO at the high temperatures being considered.

The kinetics mechanism for the calculations (shown in Appendix A) is essentially identical to that of Miller and Bowman (13), with a few species deleted to fit the constraints of the LSENS program. Additional reactions involving methanol, ethanol, and butane are taken from Westbrook and Dryer.(14) Finally, thermodynamic data has been obtained from B. J. McBride (Lewis Research Center) and the Sandia National Laboratory.(15)

Oxidation of NO in the Presence of Methanol

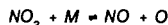
The fractional conversion of NO to NO_2 at various temperatures is shown in Fig. 2. As seen in the observations of Lyon, et al, the oxidation of NO occurs more quickly at higher temperatures.(11)

Hori (16) observed the formation of NO_2 in fuel-rich combustion and suggested that NO was oxidized by HO_2 , while a similar result was reported by Sano (17) in a calculation of a hot gas mixing with cold air. The HO_2 is predominately formed from methyl alcohol and the CH_2OH radical, both products of methanol decomposition.(11) To test these findings, the reaction:



was deleted from the model, and the NO_2 concentration was recalculated. The initial mixture composition was retained, and the initial temperature was set at 1100 K. This temperature was chosen because it had been found previously to result in the rapid formation of NO_2 . With the above reaction removed, however, the formation of NO_2 was now negligible; but, when the forward reaction was restored but not the reverse reaction, significant NO_2 formation again took place. Hence, NO oxidation is dependent on: 1) the formation of HO_2 , and 2) the reaction between HO_2 and NO.

Once all of the alcohol is consumed, NO_2 reverts to NO. This follows from the reactions involved in the chemical reduction of NO_2 :



By varying the rates for the above reactions, it was found that all but the first reaction can reduce the NO_2 concentration. When methanol is consumed, these reactions act to lower the NO_2 concentration. The activity of the reactions also explains why NO_2 concentration is lower at higher temperatures.

To determine if the concentration of methanol has any effect on NO oxidation, the oxidation process was examined at different concentrations of CH_2OH using 1100 K as the reaction temperature. It appears that, in the presence of large amounts of methanol, the speed of the oxidation process increases. Heat is released in such cases, and it has already been noted that NO oxidation occurs more quickly at higher temperatures. However, if the amount of excess methanol is small, the rate of oxidation is not affected. Understandably, since their work did not consider mixtures with large amounts of methanol, Lyon, et al, reported only this latter finding.(11)

The effect of oxygen on NO oxidation in the presence of methanol was also studied. It was determined that increases in O_2 concentration do not affect the rate.

Oxidation of NO in the Presence of Ethanol

Since ethanol and methanol are very similar chemically, it can be expected that ethanol will behave similarly in

the oxidation of NO. Unfortunately, there is no experimental data available; therefore, the choice of the kinetic model is very important to insure the accuracy of the analysis. The mechanism of Westbrook and Dryer was chosen, as it was found to have rate parameters that were very similar to those of the methanol mechanism.

The calculations made with this mechanism showed that ethanol oxidizes NO to NO₂ in a manner identical to methanol. The variations in NO₂ concentration with time and temperature are shown in Fig. 3. As expected, NO₂ formation initially rises with increasing temperature and then falls as the ethanol is consumed.

Oxidation of NO in the Presence of Ethane and Butane

Little experimental data is available on the oxidation of NO in the presence of hydrocarbons. Hori (16) found that, as with methanol and ethanol, hydrocarbon reactions also generate HO₂, while Malte and Kramlich (18) also saw evidence of NO₂ formation. In a similar situation, Jasma and Boreman (19) showed that small amounts of H₂ and CO led to NO to NO₂ conversion, while the first author (20) has demonstrated the use of methane and hydrogen to also promote NO oxidation. Thus, the presence of ethane and butane might boost NO oxidation.

Figs. 4 and 5 show the calculated NO₂ concentration at varying temperatures in the presence of ethane and butane, respectively. As with methanol, the major species involved in the oxidation of NO is HO₂. This was proved using a method similar to that followed in the case of methanol. In fact, it was found that ethane and methanol behave almost identically in the oxidation of NO. When a large amount of ethane is present, there is some reduction of the total NO_x, and the reduction increases at higher temperatures. This reduction is due to reactions involving hydrocarbon fragments.

The effect of adding large amounts of oxygen was also studied. As the oxygen concentration varied from 4% to 12%, NO₂ formation changed by only 10%.

Conclusions

Computer modeling has been used to study the formation of NO in the presence of methanol, ethanol, butane, and ethane. It appears that NO₂ is formed through oxidation of NO by HO₂, which is generated by these additives. The oxidation process is temperature dependent, with higher conversion rates at higher temperatures. However, at all temperatures, the NO₂ begins to revert to NO, once the additives are consumed; but, as long as the additives are present, the oxidation rate is only slightly dependent on the actual additive concentration. Although the presence of oxygen is necessary for the formation of NO₂, excess oxygen does not affect the NO₂ conversion.

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Table I. Initial Mixture Composition.

Species	Mole Fraction	Species	Mole Fraction
O ₂	0.0400	NO	0.0002
CH ₃ OH	0.0004	CO ₂	0.0100
H ₂ O	0.1000	Ar	0.0080
N ₂	0.8414		

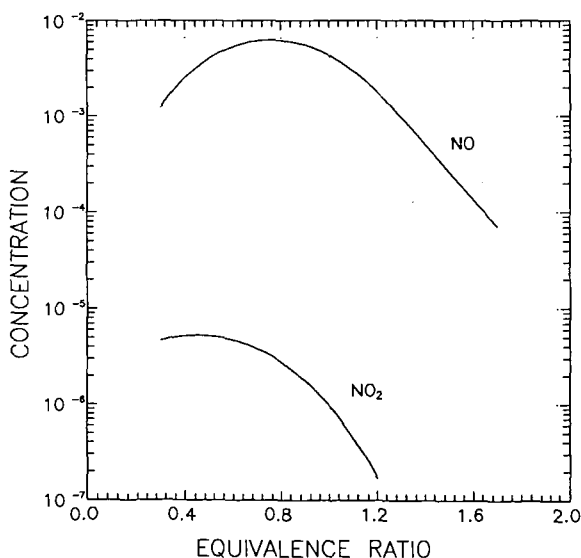


Figure 1. Equilibrium NO and NO₂ Concentrations (T = 800 K, p = 1 atm).

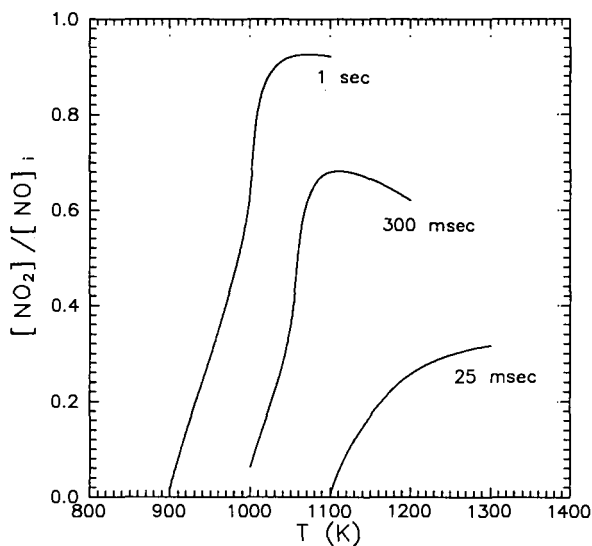


Figure 2. NO Conversion In the Presence of Methanol.

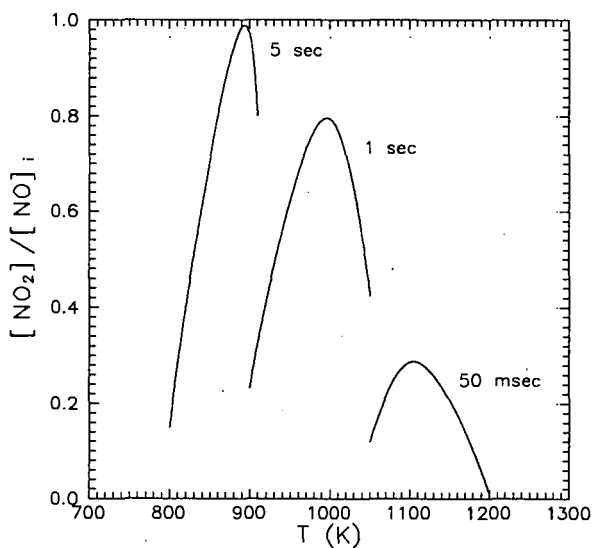


Figure 3. NO Conversion In the Presence of Ethanol.

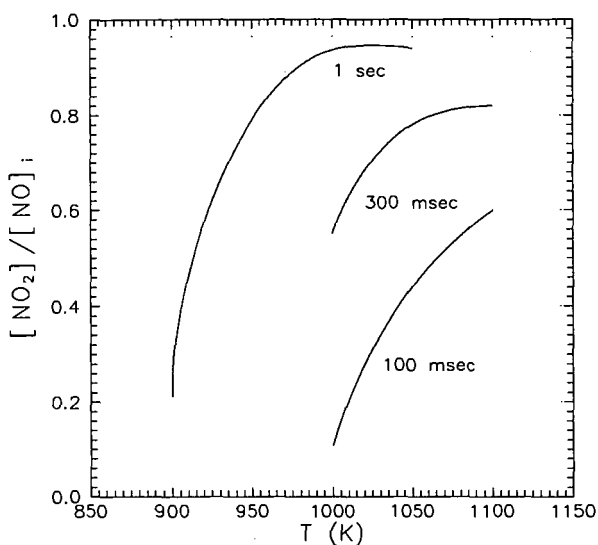


Figure 4. NO Conversion In the Presence of Ethane.

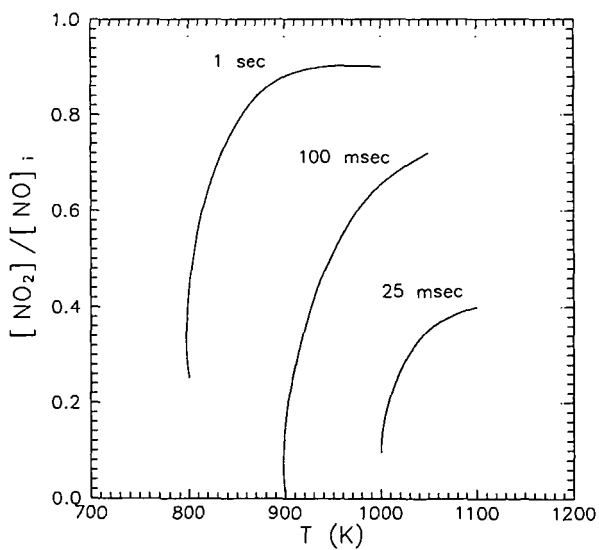


Figure 5. NO Conversion In the Presence of Butane.

Appendix A. Kinetics Mechanism.(13)

$$k = A T^B e^{-C/RT}$$

REACTION	A	B	C	REACTION	A	B	C
$M + 2CH_3 \rightarrow C_2H_6 + M$	9.03×10^{16}	-1.2	654.0	$CH + CH_2 \rightarrow C_2H_2 + H$	4.00×10^{13}	0.0	0.0
CO 2.0, H ₂ 2.0, CO ₂ 3.0, H ₂ O 5.0				$CH + CH_3 \rightarrow C_2H_3 + H$	3.00×10^{13}	0.0	0.0
$CH_3 + H \rightarrow CH_4 + M$	6.00×10^{16}	-1.0	0.0	$CH + CH_4 \rightarrow C_2H_4 + H$	6.00×10^{13}	0.0	0.0
CO 2.0, H ₂ 2.0, CO ₂ 3.0, H ₂ O 5.0				$C + O_2 \rightarrow CO + O$	2.00×10^{13}	0.0	0.0
$CH_4 + O_2 \rightarrow CH_3 + HO_2$	7.90×10^{13}	0.0	56000.0	$C + OH \rightarrow CO + H$	5.00×10^{13}	0.0	0.0
$CH_4 + H \rightarrow CH_3 + H_2$	2.20×10^{04}	3.0	8750.0	$C + CH_3 \rightarrow C_2H_2 + H$	5.00×10^{13}	0.0	0.0
$CH_4 + OH \rightarrow CH_3 + H_2O$	1.60×10^{06}	2.1	2460.0	$C + CH_2 \rightarrow C_2H + H$	5.00×10^{13}	0.0	0.0
$CH_4 + O \rightarrow CH_3 + OH$	1.02×10^{09}	1.5	8604.0	$CH_2 + CO_2 \rightarrow CH_2O + CO$	1.10×10^{11}	0.0	1000.0
$CH_4 + HO_2 \rightarrow CH_3 + H_2O_2$	1.80×10^{11}	0.0	18700.0	$CH_2 + O \rightarrow 2H + CO$	5.00×10^{13}	0.0	0.0
$CH_3 + HO_2 \rightarrow CH_3O + OH$	2.00×10^{13}	0.0	0.0	$CH_2 + O \rightarrow CO + H_2$	3.00×10^{13}	0.0	0.0
$CH_3 + O_2 \rightarrow CH_3O + O$	2.05×10^{19}	-1.6	29229.0	$CH_2 + O_2 \rightarrow 2H + CO_2$	1.60×10^{12}	0.0	1000.0
$CH_3 + O \rightarrow CH_2O + H$	8.00×10^{13}	0.0	0.0	$CH_2 + O_2 \rightarrow CH_2O + O$	5.00×10^{13}	0.0	9000.0
$CH_2OH + H \rightarrow CH_3 + OH$	1.00×10^{14}	0.0	0.0	$CH_2 + O_2 \rightarrow CO + H_2O$	1.90×10^{10}	0.0	-1000.0
$M + CH_2OH \rightarrow CH_2O + H$	1.00×10^{14}	0.0	25000.0	$CH_2 + O_2 \rightarrow CO_2 + H_2$	6.90×10^{11}	0.0	500.0
$CH_2OH + H \rightarrow CH_2O + H_2$	2.00×10^{13}	0.0	0.0	$CH_2 + O_2 \rightarrow HCO + OH$	4.30×10^{10}	0.0	-500.0
$CH_2OH + OH \rightarrow CH_2O + H_2O$	1.00×10^{13}	0.0	0.0	$CH_2O + OH \rightarrow HCO + H_2O$	3.43×10^{09}	1.18	-447.0
$CH_2OH + O \rightarrow CH_2O + OH$	1.00×10^{13}	0.0	0.0	$CH_2O + H \rightarrow HCO + H_2$	2.19×10^{08}	1.77	3000.0
$CH_2OH + O_2 \rightarrow CH_2O + HO_2$	1.48×10^{13}	0.0	1500.0	$M + CH_2O \rightarrow HCO + H$	3.31×10^{16}	0.0	81000.0
$M + CH_3OH \rightarrow CH_3 + OH$	3.02×10^{18}	0.0	80000.0	$CH_2O + O \rightarrow HCO + OH$	1.80×10^{13}	0.0	3080.0
$H + CH_3OH \rightarrow CH_3 + H_2O$	2.00×10^{12}	0.0	5300.0	$HCO + OH \rightarrow H_2O + CO$	1.00×10^{14}	0.0	0.0
$H + CH_3OH \rightarrow CH_2OH + H_2$	3.02×10^{13}	0.0	7000.0	$M + HCO \rightarrow H + CO$	2.50×10^{14}	0.0	16802.0
$OH + CH_3OH \rightarrow CH_2OH + H_2O$	3.98×10^{12}	0.0	2000.0	CO 1.9, H ₂ 1.9, CH ₄ 2.8, CO ₂ 3.0, H ₂ O 5.0			
$CH_3O + H \rightarrow CH_3 + OH$	1.00×10^{14}	0.0	0.0	$HCO + H \rightarrow CO + H_2$	1.19×10^{13}	0.25	0.0
$CH_3OH + O_2 \rightarrow CH_2OH + HO_2$	3.98×10^{10}	0.0	50910.0	$HCO + O \rightarrow CO + OH$	3.00×10^{13}	0.0	0.0
$CH_3OH + O \rightarrow CH_2OH + OH$	1.70×10^{12}	0.0	2290.0	$HCO + O \rightarrow CO_2 + H$	3.00×10^{13}	0.0	0.0
$CH_3OH + CH_3 \rightarrow CH_2OH + CH_4$	1.82×10^{11}	0.0	9800.0	$HCO + O_2 \rightarrow HO_2 + CO$	3.00×10^{13}	0.0	0.0
$CH_3OH + HO_2 \rightarrow CH_2OH + H_2O_2$	6.31×10^{12}	0.0	19360.0	$CO + O \rightarrow CO_2 + M$	6.17×10^{14}	0.0	3000.0
$CH_3 + OH \rightarrow CH_2 + H_2O$	7.50×10^{06}	2.0	5000.0	$CO + OH \rightarrow CO_2 + H$	1.51×10^{07}	1.3	-758.0
$CH_3 + H \rightarrow CH_2 + H_2$	9.00×10^{13}	0.0	15100.0	$CO + O_2 \rightarrow CO_2 + O$	1.60×10^{13}	0.0	41000.0
$M + CH_3O \rightarrow CH_2O + H$	1.00×10^{14}	0.0	25000.0	$HO_2 + CO \rightarrow CO_2 + OH$	5.80×10^{13}	0.0	22934.0
$CH_3O + H \rightarrow CH_2O + H_2$	2.00×10^{13}	0.0	0.0	$C_2H_6 + CH_3 \rightarrow C_2H_5 + CH_4$	5.50×10^{-01}	4.0	8300.0
$CH_3O + OH \rightarrow CH_2O + H_2O$	1.00×10^{13}	0.0	0.0	$C_2H_6 + O_2 \rightarrow C_2H_5 + HO_2$	1.00×10^{13}	0.0	51000.0
$CH_3O + O \rightarrow CH_2O + OH$	1.00×10^{13}	0.0	0.0	$C_2H_6 + H \rightarrow C_2H_5 + H_2$	5.40×10^{02}	3.5	5210.0
$CH_3O + O_2 \rightarrow CH_2O + HO_2$	6.30×10^{10}	0.0	2600.0	$C_2H_6 + O \rightarrow C_2H_5 + OH$	2.51×10^{13}	0.0	6360.0
$CH_2 + H \rightarrow CH + H_2$	1.00×10^{18}	-1.56	0.0	$C_2H_6 + OH \rightarrow C_2H_5 + H_2O$	8.70×10^{09}	1.05	1810.0
$CH_2 + OH \rightarrow CH + H_2O$	1.13×10^{07}	2.0	3000.0	$C_2H_4 + H \rightarrow C_2H_3 + H_2$	1.10×10^{14}	0.0	8500.0
$CH_2 + OH \rightarrow CH_2O + H$	2.50×10^{13}	0.0	0.0	$C_2H_4 + O \rightarrow CH_3 + HCO$	3.32×10^{12}	0.0	1130.0
$CH + O_2 \rightarrow HCO + O$	3.30×10^{13}	0.0	0.0	$C_2H_4 + OH \rightarrow C_2H_3 + H_2O$	2.02×10^{13}	0.0	5955.0
$CH + O \rightarrow CO + H$	5.70×10^{13}	0.0	0.0	$CH_2 + CH_3 \rightarrow C_2H_4 + H$	3.00×10^{13}	0.0	0.0
$CH + OH \rightarrow HCO + H$	3.00×10^{13}	0.0	0.0	$M + C_2H_5 \rightarrow C_2H_4 + H$	2.00×10^{15}	0.0	30000.0
$CH + CO_2 \rightarrow HCO + CO$	3.40×10^{12}	0.0	690.0	$C_2H_5 + H \rightarrow 2CH_3$	1.00×10^{14}	0.0	0.0
$CH + H \rightarrow C + H_2$	1.50×10^{14}	0.0	0.0	$C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$	8.43×10^{11}	0.0	3875.0
$CH + H_2O \rightarrow CH_2O + H$	1.17×10^{15}	-0.75	0.0	$C_2H_2 + O \rightarrow CH_3 + CO$	1.02×10^{07}	2.0	1900.0
$CH + CH_2O \rightarrow CH_2CO + H$	9.46×10^{13}	0.0	-515.0	$C_2H_2 + O \rightarrow HCCO + H$	1.02×10^{07}	2.0	1900.0

REACTION	A	B	C	REACTION	A	B	C
$C_2H_2 + O_2 \rightarrow 2HCO$	3.98×10^{12}	0.0	28000.0	$OH + HO_2 \rightarrow H_2O + O_2$	7.50×10^{12}	0.0	0.0
$H_2 + C_2H \rightarrow C_2H_2 + H$	1.02×10^{07}	2.0	1900.0	$H + HO_2 \rightarrow 2OH$	1.40×10^{14}	0.0	1073.0
$H + C_2H_2 \rightarrow C_2H_3 + M$	5.54×10^{12}	0.0	2410.0	$O + HO_2 \rightarrow O_2 + OH$	1.40×10^{13}	0.0	1073.0
H_2 2.0, CO 2.0, CO_2 3.0, H_2O 5.0				$2OH \rightarrow O + H_2O$	6.00×10^{08}	1.3	0.0
$C_2H_3 + H \rightarrow C_2H_2 + H_2$	4.00×10^{13}	0.0	0.0	$M + 2H \rightarrow H_2 + M$	1.00×10^{18}	-1.0	0.0
$C_2H_3 + O \rightarrow CH_2CO + H$	3.00×10^{13}	0.0	0.0	$H_2 + 2H \rightarrow 2H_2$	9.20×10^{16}	-0.6	0.0
$C_2H_3 + O_2 \rightarrow C_2H_2 + HO_2$	1.00×10^{12}	0.0	10000.0	$H_2O + 2H \rightarrow H_2 + H_2O$	6.00×10^{19}	-1.2	0.0
$C_2H_3 + O_2 \rightarrow CH_2O + HCO$	4.00×10^{12}	0.0	-250.0	$H + OH \rightarrow H_2O + M$	1.60×10^{22}	-2.0	0.0
$C_2H_3 + OH \rightarrow C_2H_2 + H_2O$	5.00×10^{12}	0.0	0.0	H_2O 5.0			
$C_2H_3 + CH_2 \rightarrow C_2H_2 + CH_3$	3.00×10^{13}	0.0	0.0	$H + O \rightarrow OH + M$	6.20×10^{16}	-0.6	0.0
$C_2H_3 + C_2H \rightarrow 2C_2H_2$	3.00×10^{13}	0.0	0.0	H_2O 5.0			
$C_2H_3 + CH \rightarrow CH_2 + C_2H_2$	5.00×10^{13}	0.0	0.0	$M + 2O \rightarrow O_2 + M$	1.89×10^{13}	0.0	-1788.0
$OH + C_2H_2 \rightarrow C_2H + H_2O$	3.37×10^{07}	2.0	14000.0	$H + HO_2 \rightarrow H_2 + O_2$	1.25×10^{13}	0.0	0.0
$OH + C_2H_2 \rightarrow CH_2CO + H$	2.18×10^{-04}	4.5	-1000.0	$2HO_2 \rightarrow H_2O_2 + O_2$	2.00×10^{12}	0.0	0.0
$OH + C_2H_2 \rightarrow CH_3 + CO$	4.83×10^{-04}	4.0	-2000.0	$M + H_2O_2 \rightarrow 2OH + M$	1.30×10^{17}	0.0	45500.0
$C_2H_2 + O \rightarrow C_2H + OH$	3.16×10^{15}	-0.6	15000.0	$H_2O_2 + H \rightarrow HO_2 + H_2$	1.60×10^{12}	0.0	3800.0
$CH_2CO + O \rightarrow CO_2 + CH_2$	1.75×10^{12}	0.0	1350.0	$H_2O_2 + OH \rightarrow H_2O + HO_2$	1.00×10^{13}	0.0	1800.0
$CH_2CO + H \rightarrow CH_3 + CO$	1.13×10^{13}	0.0	3428.0	$NO_2 + O \rightarrow NO + O_2$	1.00×10^{13}	0.0	600.0
$CH_2CO + H \rightarrow HCCO + H_2$	5.00×10^{13}	0.0	8000.0	$M + NO_2 \rightarrow NO + O$	1.10×10^{16}	0.0	66000.0
$CH_2CO + O \rightarrow HCCO + OH$	1.00×10^{13}	0.0	8000.0	$NH + O_2 \rightarrow HNO + O$	1.00×10^{13}	0.0	12000.0
$CH_2CO + OH \rightarrow HCCO + H_2O$	7.50×10^{12}	0.0	2000.0	$NH + O_2 \rightarrow NO + OH$	7.60×10^{10}	0.0	1530.0
$M + CH_2CO \rightarrow CH_2 + CO$	3.00×10^{14}	0.0	70980.0	$NH + NO \rightarrow N_2O + H$	2.40×10^{15}	-0.8	0.0
$C_2H + O_2 \rightarrow 2CO + H$	5.00×10^{13}	0.0	1500.0	$H_2O + H \rightarrow H_2 + OH$	7.60×10^{13}	0.0	15200.0
$H + HCCO \rightarrow CH_2 + CO$	1.00×10^{14}	0.0	0.0	$M + N_2O \rightarrow N_2 + O$	1.62×10^{14}	0.0	51600.0
$O + HCCO \rightarrow 2CO + H$	1.00×10^{14}	0.0	0.0	$H_2O + O \rightarrow H_2 + O_2$	1.00×10^{14}	0.0	28200.0
$HCCO + O_2 \rightarrow 2.0CO + OH$	1.60×10^{12}	0.0	854.0	$H_2O + O \rightarrow 2HO$	1.00×10^{14}	0.0	28200.0
$CH + HCCO \rightarrow C_2H_2 + CO$	5.00×10^{13}	0.0	0.0	$H_2O + OH \rightarrow H_2 + HO_2$	2.00×10^{12}	0.0	10000.0
$2HCCO \rightarrow 2CO + C_2H_2$	1.00×10^{13}	0.0	0.0	$NH + OH \rightarrow HNO + H$	2.00×10^{13}	0.0	0.0
$C_2H + O \rightarrow CH + CO$	5.00×10^{13}	0.0	0.0	$NH + OH \rightarrow N + H_2O$	5.00×10^{11}	0.5	2000.0
$C_2H + OH \rightarrow HCCO + H$	2.00×10^{13}	0.0	0.0	$NH + N \rightarrow H_2 + H$	3.00×10^{13}	0.0	0.0
$2CH_2 \rightarrow C_2H_2 + H_2$	4.00×10^{13}	0.0	0.0	$NH + H \rightarrow N + H_2$	1.00×10^{14}	0.0	0.0
$CH_2 + HCCO \rightarrow C_2H_3 + CO$	3.00×10^{13}	0.0	0.0	$NH + O \rightarrow NO + H$	2.00×10^{13}	0.0	0.0
$C_3H_3 + O_2 \rightarrow CH_2CO + HCO$	3.00×10^{10}	0.0	2868.0	$M + HNO \rightarrow H + NO$	1.50×10^{16}	0.0	48680.0
$C_3H_3 + O \rightarrow CH_2O + C_2H$	2.00×10^{13}	0.0	0.0	H_2O 10.0, O_2 2.0, N_2 2.0, H_2 2.0			
$C_2H_2 + O_2 \rightarrow HCCO + OH$	2.00×10^{08}	1.5	30100.0	$HNO + OH \rightarrow NO + H_2O$	3.60×10^{13}	0.0	0.0
$M + C_2H_2 \rightarrow C_2H + H$	4.20×10^{16}	0.0	107000.0	$HNO + H \rightarrow H_2 + NO$	5.00×10^{12}	0.0	0.0
$M + C_2H_2 \rightarrow C_2H_2 + H_2$	1.50×10^{15}	0.0	55800.0	$2HNO \rightarrow N_2O + H_2O$	3.95×10^{12}	0.0	5000.0
$M + C_2H_4 \rightarrow C_2H_3 + H$	1.40×10^{16}	0.0	82360.0	$HNO + NO \rightarrow N_2O + OH$	2.00×10^{12}	0.0	26000.0
$H_2 + O_2 \rightarrow 2OH$	1.70×10^{13}	0.0	47780.0	$N + NO \rightarrow N_2 + O$	3.27×10^{12}	0.3	0.0
$OH + H_2 \rightarrow H_2O + H$	1.17×10^{09}	1.3	3626.0	$N + O_2 \rightarrow NO + O$	6.40×10^{09}	1.0	6280.0
$O + OH \rightarrow O_2 + H$	4.00×10^{14}	-0.5	0.0	$N + OH \rightarrow NO + H$	3.80×10^{13}	0.0	0.0
$O + H_2 \rightarrow OH + H$	5.06×10^{04}	2.7	6290.0	$HO_2 + NO \rightarrow NO_2 + OH$	2.11×10^{11}	0.0	-479.0
$H + O_2 \rightarrow HO_2 + M$	3.61×10^{17}	-0.7	0.0	$NO_2 + H \rightarrow NO + OH$	3.50×10^{14}	0.0	1500.0
H_2O 18.6, H_2 2.9, N_2 1.3				$2NH \rightarrow 2H + N_2$	7.20×10^{13}	0.0	0.0

UNITS: A cm-mol/sec; B -; C cal/mol